WHAT IS CLAIMED IS:

1. A method for obtaining at least one calibration filter for a Mass Spectrometry (MS) instrument system, comprising the step of:

obtaining, for a given calibration standard, measured isotope peak cluster data in a mass spectral range;

calculating, for the given calibration standard, relative isotope abundances and actual mass locations of isotopes corresponding thereto;

specifying mass spectral target peak shape functions centered within respective mass spectral ranges;

performing convolution operations between the calculated relative isotope abundances and the mass spectral target peak shape functions to form calculated isotope peak cluster data; and

performing a deconvolution operation between the measured isotope peak cluster data and the calculated isotope peak cluster data after the convolution operations to obtain the at least one calibration filter.

2. The method of claim 1, wherein any of said steps of performing convolution operations and performing a deconvolution operation employs at least one of a Fourier Transform, a matrix multiplication, and a matrix inversion

3. The method of claim 1, further comprising the step of pre-aligning measured mass spectral isotope peaks based on a least squares polynomial fit between centroid masses of the

calculated relative isotope abundances and those of the measured isotope peak clusters, in a pre-calibration step performed subsequent to said calculating step.

4. The method of claim 1, further comprising the steps of:

performing pre-calibration instrument-dependent transformations on raw mass spectral data; and

performing post-calibration instrument-dependent transformations on a calculated data set corresponding to a test sample.

5. The method of claim 4, wherein said steps of performing pre-calibration instrument-dependent transformations and performing post-calibration instrument-dependent transformations involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero column along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to the pre-calibration instrument-dependent transformations and the post-calibration instrument-dependent transformations, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

6. The method of claim 5, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

7. The method of claim 6, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and the raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

8. The method of claim 7, further comprising the step of applying a weighted regression operation to calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

9. The method of claim 8, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

10. The method of claim 7, further comprising the step of applying multivariate statistical analysis to calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

11. The method of claim 1, further comprising the steps of:

performing a pre-calibration mass spacing adjustment from a non-uniformly spaced mass acquisition interval to a uniformly spaced mass interval; and

performing a post-calibration mass spacing adjustment from the uniformly spaced mass interval to a reporting interval.

12. The method of claim 11, wherein said steps of performing the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero column along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

13. The method of claim 12, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

14. The method of claim 13, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

15. The method of claim 14, further comprising the step of applying a weighted regression operation to calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

16. The method of claim 15, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

17. The method of claim 14, further comprising the step of applying multivariate statistical analysis to calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

18. The method of claim 1, wherein the at least one calibration filter comprises at least two calibration filters, and said method further comprises the step of further interpolating between the at least two calibration filters to obtain at least one other calibration filter within a desired mass range.

19. The method of claim 18, wherein said interpolating step comprises the steps of:

collecting the at least two calibration filters as vectors in a matrix for decomposition;

decomposing the matrix that includes the at least two calibration filters;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other calibration filter using the interpolated vectors.

20. The method of claim 19, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

21. The method of claim 1, further comprising the step of adding the calibration standard into a test sample one of prior to and in real-time through at least one of continuous infusion and online mixing so as to acquire both calibration data and test data in a single mass spectral acquisition.

22. A method of processing raw mass spectral data, comprising the steps of:

applying a total filtering matrix to the raw mass spectral data to obtain calibrated mass spectral data,

wherein the total filtering matrix is formed by:

measured isotope peak cluster data, obtained for a given calibration standard in a mass spectral range

relative isotope abundances and actual mass locations of isotopes corresponding thereto, calculated for a same calibration standard,

specified mass spectral target peak shape functions centered within the mass spectral range,

convolution operations performed between the calculated relative isotope abundances and the mass spectral target peak shape functions to form calculated isotope peak cluster data; and

a deconvolution operation performed between the measured isotope peak cluster data and calculated isotope peak cluster data after the convolution operations to obtain at least one calibration filter for the total filtering matrix.

23. The method of claim 22, wherein said applying step further comprises the step of interpolating the raw mass spectral data onto a same mass axis as that required by the total filtering matrix.

24. The method of claim 22, wherein said applying step further comprises the step of interpolating the calibrated mass spectral data onto any desired mass axis different from that given by the total filtering matrix.

25. The method of claim 22, further comprising the step of applying a weighted regression operation to the calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

26. The method of claim 25, wherein weights of the weighted regression operation are proportional to an inverse of mass spectral variances.

27. The method of claim 22, further comprising the step of applying multivariate statistical analysis to the calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

28. A method for analyzing mass spectral peaks corresponding to mass spectral data obtained from a Mass Spectrometry (MS) instrument system, the method comprising the steps of:

applying a weighted regression operation to mass spectral peaks within a mass spectral range; and

reporting regression coefficients as one of integrated peak areas and mass deviations corresponding to one of nominal masses and estimated actual masses.

29. The method of claim 28, wherein said method is performed subsequent to the MS instrument system being calibrated such that mass spectral peak shape functions are given by target peak shape functions.

30. The method of claim 28, wherein weights of the weighted regression operation are proportional to an inverse of mass spectral variances.

31. The method of claim 28, wherein said applying and reporting steps are repeated until incremental improvements in at least one of the integrated peak areas and the mass deviations meet preset criteria.

32. The method of claim 28, wherein said analyzing step further comprises the step of calculating standard deviations for one of the integrated peak areas and the mass deviations based on weights of the weighted regression operation and the weighted regression operation.

33. The method of claim 32, wherein said calculating step further comprises the step of calculating t-statistics for at least one of the integrated peak areas and the mass deviations, the t-statistics being adapted for testing and reporting a statistical significance of at least one of calculated peak areas and mass locations, wherein the statistical significance indicates a presence or an absence of a mass spectral peak.

34. The method of claim 28, further comprising the step of creating a peak component matrix, including calculating a pair of matrix rows, with a first row of the pair of matrix rows for storing a mass spectral peak shape function and with a second row of the pair of matrix rows for storing a first derivative of the mass spectral peak shape function stored in the first row.

35. The method of claim 34, wherein the peak shape function includes additionally at least one of linear and nonlinear functions to account for mass spectral baseline components.

36. The method of claim 34, wherein the peak shape function is one of target peak shape function and a known instrument peak shape function.

37. The method of claim 36, wherein the mass spectral peak shape function and the first derivative thereof are identical across a mass spectral range and are both sampled at a same integer fraction of a nominal mass spacing.

38. The method of claim 37, further comprising the step of completing the peak component matrix such that any mass spectral peak shape functions in any remaining matrix

rows are arranged as shifted versions of each other corresponding to each nominal mass within a mass spectral range.

39. The method of claim 34, further comprising one of:

updating nominal masses in the peak component matrix to estimated actual masses by adding reported mass deviations to the nominal masses; and

updating the estimated actual masses in the peak component matrix to further refined estimated actual masses by adding reported mass deviations to the estimated actual masses.

40. The method of claim 28, further comprising the step of interpolating data corresponding to mass spectral peak shape functions to obtain one other mass spectral peak shape function at each of the nominal masses.

41. The method of claim 40, wherein said interpolating step comprises the steps of:

collecting the mass spectral peak shape functions as vectors in a matrix for decomposition;

decomposing the mass spectral peak shape functions included in the matrix;

interpolating between decomposed vectors to obtain interpolated vectors; and

reconstructing the one other mass spectral peak shape function at each of the nominal masses using the interpolated vectors.

42. The method of claim 41, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

43. The method of claim 40, further comprising the step of calculating first derivatives of the mass spectral peak shape functions at each of the nominal masses.

44. The method of claim 43, further comprising the step of creating a peak component matrix, by combining the mass spectral peak shape functions and the first derivates corresponding thereto.

45. The method of claim 44, further comprising one of:

updating nominal masses in the peak component matrix to estimated actual masses by adding reported mass deviations to the nominal masses; and

updating the estimated actual masses in the peak component matrix to further refined estimated actual masses by adding reported mass deviations to the estimated actual masses.

46. The method of claim 44, wherein the peak component matrix includes additionally at least one of linear and nonlinear functions to account for mass spectral baseline components.

47. The method of claim 28, wherein said applying step further comprises the step of performing at least one of a matrix inversion and a matrix decomposition.

48. The method of claim 47, wherein the at least one of the matrix inversion and the matrix decomposition is based on at least one of a banded nature, a symmetrical nature, and a cyclic nature of a peak component matrix.

49. The method of claim 47, wherein results of at least one of the matrix inversion and the matrix decomposition are calculated and stored prior to analyzing test sample data.

50. A method for calculating calibration filters for a Mass Spectrometry (MS) instrument system, comprising the step of:

obtaining, from a given calibration standard, at least one mass spectral peak shape function,

specifying mass spectral target peak shape functions centered at mid points within respective mass spectral ranges,

performing a deconvolution operation between the obtained at least one mass spectral peak shape function and the mass spectral target peak shape functions, and

calculating at least one calibration filter from a result of the deconvolution operation.

51. The method of claim 50, wherein the at least one mass spectral peak shape function can be obtained from a section of a mass spectrum that contains a single significant isotope peak with no significant overlaps from other minor isotope peaks.

52. The method of claim 50, wherein said obtaining step comprises the steps of:

calculating, for the given calibration standard, relative isotope abundances and actual mass locations of the isotopes corresponding thereto;

performing convolution operations on both the calculated relative isotope abundances and measured isotope peak clusters using a same continuous function with a narrow peak width; and

performing a deconvolution operation between the measured isotope peak clusters and calculated isotope peak clusters after said convolution operations to obtain the at least one mass spectral peak shape function

53. The method of claim 50, wherein the at least one calibration filter comprises at least two calibration filters, and said method further comprises the step of further interpolating between the at least two calibration filters to obtain at least one other calibration filter within a desired mass range.

54. The method of claim 53, wherein said interpolating step comprises the steps of:

collecting the at least two calibration filters as vectors in a matrix for decomposition;

decomposing the matrix that includes the at least two calibration filters;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other calibration filter using the interpolated vectors.

55. The method of claim 54, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

56. The method of claim 50, wherein any of said steps of performing a deconvolution operation employs at least one of a Fourier Transform and a matrix inversion.

57. The method of claim 52, wherein any of said steps of performing a convolution and deconvolution operation employs at least one of a Fourier Transform, a matrix multiplication, and a matrix inversion.

58. The method of claim 50, wherein said obtaining step further comprises the step of interpolating data corresponding to the mass spectral peak shape functions to obtain at least one other mass spectral peak shape function within a desired mass range.

59. The method of claim 58, wherein said interpolating step comprises the steps of:

collecting the mass spectral peak shape functions as vectors in a matrix for decomposition;

decomposing the matrix that includes the mass spectral peak shape functions;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other mass spectral peak shape function using the interpolated vectors.

60. The method of claim 59, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

61. The method of claim 58, wherein said performing step comprises the step of performing a deconvolution operation between mass spectral target peak shape functions and one of measured mass spectral peak shape functions and the calculated mass spectral peak shape functions to convert the measured mass spectral peak shape functions and the at least one other mass spectral peak shape function to the mass spectral target peak shape functions centered at mid-points within the respective mass spectral ranges; and

wherein said calculating step comprises the step of calculating at least one calibration filter from the deconvolution operation.

62. The method of claim 61, wherein the at least one calibration filter comprises at least two calibration filters, and said method further comprises the step of further interpolating between the at least two calibration filters to obtain at least one other calibration filter within a desired mass range.

63. The method of claim 62, wherein said further interpolating step comprises the steps of:

collecting the at least two calibration filters as vectors in a matrix for decomposition;

decomposing the matrix that includes at least two calibration filters;

interpolating between decomposed vectors of the matrix to obtain interpolated vectors; and

reconstructing the at least one other calibration filter using the interpolated vectors.

64. The method of claim 63, wherein said decomposing step is performed using at least one of Singular Value Decomposition (SVD) and wavelet decomposition.

65. The method of claim 61, wherein said step of performing a deconvolution operation between the mass spectral target peak shape functions and one of the measured mass spectral peak shape functions and the calculated mass spectral peak shape functions employs at least one of a Fourier Transform and a matrix inversion.

66. The method of claim 50, further comprising the step of pre-aligning mass spectral isotope peaks based on a least squares polynomial fit between centroid masses of the calculated relative isotope abundances and those of the measured isotope peak clusters, in a pre-calibration step performed subsequent to said calculating step.

67. The method of claim 50, further comprising the steps of: performing pre-calibration instrument-dependant transformations on raw mass spectral data; and performing post-calibration instrument-dependent transformations on a calculated data set corresponding to a test sample

68. The method of claim 67, wherein said steps of performing pre-calibration instrument-dependent transformations and performing post-calibration instrument-dependent transformations involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero column along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to

the pre-calibration instrument-dependent transformations and the post-calibration instrument-dependent transformations, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

69. The method of claim 68, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

70. The method of claim 69, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and the raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

71. The method of claim 70, further comprising the step of applying a weighted regression operation to calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

72. The method of claim 71, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

73. The method of claim 70, further comprising the step of applying multivariate statistical analysis to calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

74. The method of claim 50, further comprising the steps of:

performing a pre-calibration mass spacing adjustment from a non-uniformly spaced mass acquisition interval to a uniformly spaced mass interval; and

performing a post-calibration mass spacing adjustment from the uniformly spaced mass interval to a reporting interval.

75. The method of claim 74, wherein said steps of performing the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment involve respectively creating a pre-calibration banded diagonal matrix and a post-calibration banded diagonal matrix, each nonzero column along a banded diagonal of each of the respective matrices for respectively performing an interpolation function corresponding to the pre-calibration mass spacing adjustment and the post-calibration mass spacing adjustment, and said method further comprises the step of creating from the at least one calibration filter a calibration banded diagonal matrix for performing both peak shape and mass axis calibration.

76. The method of claim 75, further comprising the step of multiplying the pre-calibration banded diagonal matrix, the calibration banded diagonal matrix and the post-calibration banded diagonal matrix into a total filtering matrix prior to calibrating a test sample.

77. The method of claim 76, wherein the peak shape and the mass axis calibration are performed by matrix multiplication between the total filtering matrix and raw mass spectral data, and said method further comprises the step of creating another banded diagonal matrix to estimate mass spectral variances of a calibrated signal, the other banded diagonal matrix having each nonzero element along a banded diagonal equal to a square of a corresponding element in the total filtering matrix.

78. The method of claim 77, further comprising the step of applying a weighted regression operation to the calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

79. The method of claim 78, wherein weights of the weighted regression operation are proportional to an inverse of the mass spectral variances.

80. The method of claim 77, further comprising the step of applying multivariate statistical analysis to the calibrated mass spectral data to at least one of quantify, identify, and classify test samples.

81. The method of claim 50, further comprising the step of adding the calibration standard into a test sample one of prior to and in real-time through at least one of continuous infusion and online mixing so as to acquire both calibration data and test data in a single mass spectral acquisition.

82. A method of processing raw mass spectral data, comprising the steps of:

applying a total filtering matrix to the raw mass spectral data to obtain calibrated mass spectral data,

wherein the total filtering matrix is formed by:

obtaining, from a given calibration standard, at least one mass spectral peak shape function,

specifying mass spectral target peak shape functions centered at mid points within respective mass spectral ranges,

performing a deconvolution operation between the obtained at least one mass spectral peak shape function and the mass spectral target peak shape functions, and

calculating at least one calibration filter from a result of the deconvolution operation.

83. The method of claim 82, wherein said applying step further comprises the step of interpolating the raw mass spectral data onto a same mass axis as that required by the total filtering matrix.

84. The method of claim 82, wherein said applying step further comprises the step of interpolating the calibrated mass spectral data onto any desired mass axis different from that given by the total filtering matrix.

85. The method of claim 82, further comprising the step of applying a weighted regression operation to the calibrated mass spectral data to obtain at least one of integrated peak areas, actual masses and other mass spectral peak data for the mass spectral peaks.

86. The method of claim 85, wherein weights of the weighted regression operation are proportional to an inverse of mass spectral variances.

87. The method of claim 82, further comprising the step of applying multivariate statistical analysis to the calibrated mass spectral data to at least one of quantify, identify, and classify test samples.